

# Analytical formula for the Uehling potential

Alexei M. Frolov\*

*Department of Applied Mathematics*

*University of Western Ontario, London, Ontario N6H 5B7, Canada*

David M. Wardlaw†

*Department of Chemistry*

*University of Western Ontario,  
London, Ontario N6H 5B7, Canada*

(Dated: March 27, 2012)

## Abstract

The closed analytical expression for the Uehling potential is derived. The Uehling potential describes the lowest-order correction on vacuum polarization in atomic and muon-atomic systems. By using our three-term analytical formula for the Uehling potential we evaluated the vacuum polarization correction(s) for the ground states in some two-electron ions. The analytical formula for the Uehling potential allows us to derive the general expression for the interaction potential between two point electric charges. This analytical formula provides the correct asymptotic behaviour at large distances between two interacting electric charges.

---

\*E-mail address: afrolov@uwo.ca

†E-mail address: dwardlaw@uwo.ca

## I. INTRODUCTION

Various effects related to the vacuum polarization in atomic systems have been analyzed by many famous theorists, including Dirac, Heisenberg, Pauli and others. A large number of fundamental papers of these authors were stimulated by investigations of the vacuum polarization problem (see, e.g. [1], [2] and [3]). Briefly, the vacuum polarization in atomic systems can be described as the creation of virtual electron-positron pairs by a photon moving in the field created by an electric charge  $eQ$  (see, e.g., [4], [5]). These virtual  $(e^-, e^+)$ -pairs will interact with the original photon, and such an interaction will affect its propagation, an effect termed the vacuum polarization by Uehling in 1935 [6]. It can be detected in all atoms and muonic atoms. For heavy atomic systems, e.g., for the Pb, Bi and U atoms and corresponding muonic atoms, the effect of vacuum polarization has been discussed in various papers (see, e.g., [7], [8] and references therein). There are some advantages in studying the effect of vacuum polarization in few-electron atoms and muonic atoms. Indeed, in the case of light atomic systems with relatively small nuclear charges  $Q \leq 10$ , we can assume that in the vicinity of an atomic nucleus with positive charge  $eQ$  the actual interaction potential will slightly be different from the scalar Coulomb potential created by the two point particles. It is found in this study that such a potential can still be written in a closed analytical form. In reality, this means that the pure Coulomb potential must be replaced by some ‘more realistic’ potential such as  $V(r) = \frac{e^2 Q}{r}(1 + f(Q, r))$ , where  $f(Q, r)$  is the function which represents the deviation of the actual potential from the Coulomb potential at small  $r$ . Note that this approach (Dirac’s approach) corresponds to the non-relativistic picture, but it can easily be generalized to the relativistic case. In general, the function  $f(Q, r)$  is determined with the use of methods of Quantum Electrodynamics. The main goal of this study is to derive the closed analytical expression for the  $f(Q, r)$  function.

The expression for the  $f(Q, r)$  function can be derived explicitly, if we know the lowest order radiative corrections to the photon Green’s function and for the vertex function. Formulas for radiative corrections to the photon Green’s function are very well known (see, e.g., [5]). By choosing the lowest order correction one obtains the modified Coulomb law in vacuum. This problem was considered for the first time by Uehling in 1935 [6] and the associated  $f(Q, r)$  function which arises in this case is called the Uehling potential. Since

early studies of vacuum polarization many different people tried to derive the closed analytical expression for the Uehling potential. Unfortunately, such an expression has not been found and it substantially delayed theoretical research of the vacuum polarization. In this study we have derived the closed, three-term analytical formula for the Uehling potential. This formula is used to obtain the properties of the Uehling potential and perform numerical evaluations of the corresponding corrections to the total energies of bound states in light two-electron atoms and ions. The closed analytical formula for the Uehling potential is the main result of this work. Note that our formula includes only three terms each of which contains either the modified Bessel function of the zero order  $K_0(2br)$ , or the recursive integrals of this function, i.e. the  $Ki_1(2br)$  and  $Ki_2(2br)$  functions. This formula provides numerous advantages for theoretical analysis as well as for numerical computations.

Note, however, that the Uehling potential has wrong long-range asymptotics, i.e. its behaviour at large  $r$  is not correct. Therefore, it must be modified to represent the interaction between the two point electric charges correctly at arbitrary, in principle, interparticle distances. This problem has substantial scientific and methodological interest. Indeed, in classical electrodynamics the interaction  $V$  between two point electric charges  $q_1e$  and  $q_2e$  is described by the Coulomb law, i.e.  $V \simeq \frac{q_1q_2e^2}{r_{12}}$ . This expression for  $V$  does not change its form in the non-relativistic quantum mechanics [9], when the Planck constant  $\hbar$  is finite. However, if we also assume that the speed of light  $c$  is finite, then Quantum Electrodynamics leads us to the necessity to modify the Coulomb law. The main correction is related to the vacuum polarization in the spatial areas close to the electric charges. In the lowest order approximation such a correction is represented by the Uehling potential [6], which is correct at short interparticle distances. However, the Uehling potential does not provide the correct long-range asymptotics, i.e. its behaviour at large  $r$  is not correct. Therefore, it must be modified to represent the interaction between the two point electric charges correctly at arbitrary, in principle, interparticle distances. This problem has substantial scientific and methodological interest. In particular, the Coulomb potential modified by a number of additional terms, which represent small QED-corrections, can be used directly in the highly accurate calculations of few-electron atoms and ions. On the other hand, it is interesting to see the transformation of the usual Coulomb potential under the rules of modern Quantum Electrodynamics.

The explicit derivation of such a corrected Coulomb potential modified by a number

additional terms is the second goal of this study. Such a potential can directly be used in highly accurate calculations of few-electron atoms and ions. On the other hand, it is interesting to see the transformation of the usual Coulomb potential under the rules of modern Quantum Electrodynamics.

## II. UEHLING POTENTIAL

As mentioned above, in the lowest order approximation the vacuum polarization is described by the Uehling potential [6] which is represented as a small, short-range correction to the regular Coulomb potential acting between the two point particles which have electric charges  $e$  and  $Qe$ . Formally, the contribution from such a correction can be represented as  $\alpha Q(r)$ , where  $\alpha = \frac{e^2}{4\pi\hbar c}$  is the fine structure constant and  $Q(r)$  is the regular Coulomb potential acting between two charged particles. The explicit formula for the Uehling potential is derived by computing the lowest-order radiative corrections to the photon Green's function. In fact, if the current  $J_\nu(x)$  is known (here and below  $\nu = 0, 1, 2, 3$ ), then the electromagnetic field  $F_\nu(x)$  which is created by this current is obtained from the following formula

$$F_\nu(x) = i \int G_{\mu\nu}^{(\gamma)}(x - x') J_\mu(x') dx' \quad (1)$$

where  $G_{\mu\nu}^{(\gamma)}(x)$  is the photon Green's function which also contains the lowest order radiative correction. The integration in Eq.(1) is performed over all 4-dimensional Minkovskii space where we have  $g_{\mu\mu} = (1, -1, -1, -1)$  and  $g_{\mu\nu} = 0$ , if  $\mu \neq \nu$ .

If the field is created by a point electric charge which is at rest, then  $J_\nu = ieQ\delta_{\nu 0}\delta(\mathbf{r})$  and the corresponding expression for scalar potential  $\phi(r)$  takes the form

$$\phi(r) = ieQ \int_{-\infty}^{\infty} G^{(\gamma)}(x) dt = \frac{ieQ}{(2\pi)^3} \int G^{(\gamma)}(\mathbf{k}, 0) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3\mathbf{k} \quad (2)$$

where  $x = (ct, \mathbf{r})$  and the last integral is a three-dimensional integral over  $\mathbf{k}$ -space. Here we designate  $\phi(r) = J_0(\mathbf{r}) = J_0(r)$ , where  $r = |\mathbf{r}|$ . The analytical formula for the  $G^{(\gamma)}(\mathbf{k}, 0)$  function is well known (see, e.g., [5] and references therein)

$$G^{(\gamma)}(\mathbf{k}, 0) = -\frac{i}{k^2} \left\{ 1 + \frac{2\alpha}{\pi} \int_0^1 x(1-x) \cdot \ln \left[ 1 + \frac{k^2}{m^2} x(1-x) \right] dx \right\} \quad (3)$$

where  $\alpha = \frac{e^2}{4\pi\hbar c}$  is the fine structure constant. In the relativistic units with  $c = 1$  and

$\hbar = 1, \alpha = \frac{e^2}{4\pi}$ . By substituting this expression in Eq.(2) one finds the formula

$$\phi(r) = \frac{eQ}{4\pi r} + \frac{Qe\alpha}{\pi(2\pi)^3} \int_0^1 \frac{v^2(1 - \frac{1}{3}v^2)}{1 - v^2} dv \int \frac{\exp(i\mathbf{k} \cdot \mathbf{r})}{k^2 + \frac{4m^2}{1-v^2}} d^3\mathbf{k} \quad (4)$$

where  $v = 2x - 1$ . The integral over the  $\mathbf{k}$  variable in this formula is

$$\int \frac{\exp(i\mathbf{k} \cdot \mathbf{r})}{k^2 + \frac{4m^2}{1-v^2}} d^3\mathbf{k} = \frac{2\pi^2}{r} \exp\left(-\frac{2mr}{\sqrt{1-v^2}}\right) \quad (5)$$

Therefore, the potential  $\phi(r)$  in Eq.(4) can be written in the form

$$\phi(r) = \frac{Qe}{4\pi r} + \frac{Qe\alpha}{4\pi^2 r} \int_0^1 \frac{v^2(1 - \frac{1}{3}v^2)}{1 - v^2} \exp\left(-\frac{2mr}{\sqrt{1-v^2}}\right) dv \quad (6)$$

where we have used the fact that the expression under the integral is an even function of  $v$ .

The integral in Eq.(6) can be transformed by introducing the new variable  $\xi = \frac{1}{\sqrt{1-v^2}}$ . From the definition of this variable  $\xi$  one finds

$$1 - \frac{1}{3}v^2 = \frac{2}{3}\left(1 + \frac{1}{2\xi^2}\right) \quad (7)$$

and

$$dv = \frac{(1 - v^2)^{\frac{3}{2}}}{v} d\xi = \frac{d\xi}{\xi^2 \sqrt{\xi^2 - 1}} \quad (8)$$

By using these formulas we reduce the integral from Eq.(6)

$$\frac{Qe\alpha}{4\pi^2 r} \int_0^1 \frac{v^2(1 - \frac{1}{3}v^2)}{1 - v^2} \exp\left(-\frac{2mr}{\sqrt{1-v^2}}\right) dv \quad (9)$$

to the form

$$\frac{\alpha Qe}{4\pi^2} \frac{2}{3} \int_1^\infty \exp(-2mr\xi) \left(1 + \frac{1}{2\xi^2}\right) \frac{\sqrt{\xi^2 - 1}}{\xi^2} d\xi \quad (10)$$

where  $\alpha = \frac{e^2}{4\pi}$  is the fine structure constant (in relativistic units). The sum of Eq.(10) with the Coulomb potential  $\frac{Qe}{4\pi r}$  is

$$\phi(r) = \frac{Qe}{4\pi r} \left[1 + \frac{2\alpha}{3\pi} \int_1^\infty \exp(-2mr\xi) \left(1 + \frac{1}{2\xi^2}\right) \frac{\sqrt{\xi^2 - 1}}{\xi^2} d\xi\right] \quad (11)$$

The energy of an elementary charge  $e$  in the field of this potential is written in the form

$$e\phi(r) = \alpha \frac{Q}{r} \left[1 + \frac{2\alpha}{3\pi} \int_1^\infty \exp(-2m\xi r) \left(1 + \frac{1}{2\xi^2}\right) \frac{\sqrt{\xi^2 - 1}}{\xi^2} d\xi\right] \quad (12)$$

In the case of atomic systems, where  $m = m_e$ , one finds the following expression for the  $ec\phi(r)$  interaction energy (in atomic units  $\hbar = 1, m_e = 1$  and  $e = 1$ )

$$ec\phi(r) = \frac{Q}{r} \left[1 + \frac{2\alpha}{3\pi} \cdot \int_1^{+\infty} \exp(-2\alpha^{-1}\xi r) \left(1 + \frac{1}{2\xi^2}\right) \frac{\sqrt{\xi^2 - 1}}{\xi^2} d\xi\right] = \frac{Q}{r} + U(r) \quad (13)$$

where  $Q$  is the integer product of two particle charges,  $c\phi$  is the 0-component of the 4-dimensional vector-potential  $A_\mu = (c\phi, \mathbf{A})$  and  $\alpha$  is the fine structure constant ( $\alpha^{-1} \approx 137.03599911$ , see, e.g., [10]). The ‘additional’ potential energy  $U(r)$  in Eq.(13) corresponds to the contribution from the so-called Uehling potential which is generated by the lowest order radiative correction to the electrodynamic Green’s function, or photon Green’s function, for short. As follows from Eq.(13) the Uehling potential differs from zero only for very short distances  $r \leq \Lambda_e$ , where  $\Lambda_e = \frac{\hbar}{m_e c} = \alpha a_0 \approx 3.861592 \cdot 10^{-11} \text{ cm}$  is the Compton wavelength of the electron and  $a_0$  is the Bohr radius.

In our derivation of analytical formulas for the  $U(r)$  term in Eq.(13) all important details are shown explicitly. The formulas given above allow one to understand some mistakes/misprints which are often made in the consideration of the Uehling potential. For instance, the integral representation (Laplace transform) of the Uehling potential given in [7] contains an extra negative power of the  $\xi$ -variable. However, our main goal below is to derive and discuss the closed analytical expression for the Uehling potential. According to the modern scientific literature such a formula does not exist and only the corresponding integral transformations are used in actual applications.

### A. Long-range and short-range asymptotics of the Uehling potential

As is well known (see, e.g., [5] and references therein) the integral

$$I = \int_1^\infty \exp(-2m\xi r) \left(1 + \frac{1}{2\xi^2}\right) \frac{\sqrt{\xi^2 - 1}}{\xi^2} d\xi \quad (14)$$

can be computed analytically for very small and very large values of its parameter  $mr$ . For  $mr \ll 1$  the approximate value of this integral is

$$I \simeq -\frac{5}{6} - \gamma - \ln(mr) \quad (15)$$

or, for  $m = m_e$  and in atomic units

$$I \simeq -\frac{5}{6} - \gamma + \ln \alpha - \ln r \approx -6.33079265675 - \ln r \quad (16)$$

where  $\gamma \approx 0.5772156649 \dots$  is the Euler constant (see, e.g., [11]) and  $\ln \alpha \approx -4.92024365857$ .

In the opposite case, i.e. when  $mr \gg 1$  the long-range asymptotics of the integral  $I$ , Eq.(14), is

$$I \simeq \frac{3\sqrt{\pi}}{8} \cdot \frac{\exp(-2mr)}{(mr)^{\frac{3}{2}}} \quad (17)$$

or, for  $m = m_e$  and in atomic units

$$I \simeq \frac{3\sqrt{\pi}}{8} \cdot \alpha^{\frac{3}{2}} \cdot \frac{\exp(-2\alpha^{-1}r)}{r^{\frac{3}{2}}} \approx 4.1433745897 \cdot 10^{-4} \cdot \frac{\exp(-2\alpha^{-1}r)}{r^{\frac{3}{2}}} \quad (18)$$

where  $\alpha^{-1} \approx 137.03599911$  (see, e.g., [10]).

By using these formulas for  $I(r)$  we can find the appropriate analytical expressions for the long-range and short-range asymptotics of the Uehling potential  $U(r)$  and its sum with the Coulomb potential. Indeed, the Uehling potential is  $U(r) = \frac{2\alpha Q}{3\pi r} I(r)$ , while for the total interaction potential we have  $\phi(r) = \frac{Q}{r} \left[ 1 + \frac{2\alpha}{3\pi} I(r) \right]$ . Here and everywhere below in this work we shall apply only atomic units. From these expressions one can find the explicit short-range and long-range asymptotics of the  $U(r)$  and  $\phi(r)$  potentials. Note that these asymptotic formulas for the  $U(r)$  potential have been known since the middle of 1930's [6] (see discussion in [18]). A number of people tried to produce the general formula for the Uehling potential. Such a formula must provide the correct asymptotics at large  $r$  and small  $r$ . All such attempts were unsuccessful and around the middle of 1950's it was finally assumed that simple analytical expression for the Uehling potential  $U(r)$  at arbitrary interparticle distances  $r$  does not exist. Since then only numerical methods are used for actual atomic and muon atomic systems. In the next Section we derive the explicit analytical formula for the Uehling potential  $U(r)$  for all values of  $r$ .

### III. ANALYTICAL FORMULA FOR THE UEHLING POTENTIAL

In numerous books and textbooks on Quantum Electrodynamics (see, e.g., [5], [13]) one can find a statement that the integral in Eq.(13) ‘cannot be evaluated in closed form but is easily solved numerically’. In other words, it is widely assumed that the analytical expression for the  $U(r)$  potential does not exist. In order to show that this statement is incorrect we proceed to obtain the closed analytical form for the Uehling potential  $U(r)$ . First, consider the following integral

$$I_U(a) = \int_1^{+\infty} \exp(-a\xi) \left( 1 + \frac{1}{2\xi^2} \right) \frac{\sqrt{\xi^2 - 1}}{\xi^2} d\xi \quad , \quad (19)$$

where  $a$  is some positive numerical parameter. By using the substitution  $\xi = \cosh x$  we reduce  $I_U$  to the form

$$I_U = \int_0^{+\infty} \exp(-a \cosh x) \left( 1 - \frac{1}{2 \cosh^2 x} - \frac{1}{2 \cosh^4 x} \right) dx = K_0(a) - \frac{1}{2} K_{i_2}(a) - \frac{1}{2} K_{i_4}(a) \quad (20)$$

where  $K_0(a)$  is the modified Bessel function of zero order, i.e.

$$K_0(z) = \int_0^\infty \exp(-z \cosh t) dt = \sum_{k=0}^{\infty} (\psi(k+1) + \ln 2 - \ln z) \frac{z^{2k}}{2^{2k} (k!)^2} ,$$

where  $\psi(k)$  is the Euler *psi*-function defined by Eq.8.362 from [11]. The functions  $Ki_2(z)$  and  $Ki_4(z)$  in Eq.(20) are the recursive integrals of the  $K_0(z)$  function, i.e.

$$Ki_1(z) = \int_z^\infty Ki_0(z) dz , \quad \text{and} \quad Ki_n(z) = \int_z^\infty Ki_{n-1}(z) dz , \quad (21)$$

where  $n \geq 1$  and  $Ki_0(z) \equiv K_0(z)$ . By using the relation given by Eq.11.2.14 from [19] for the recursive integrals  $Ki_n(z)$  (where  $n \geq 0$ ) one can reduce Eq.(20) to the following form

$$I_U(z) = \left(1 + \frac{z^2}{12}\right) K_0(z) - \frac{z}{12} Ki_1(z) + \left(\frac{5}{6} - \frac{z^2}{12}\right) Ki_2(z) . \quad (22)$$

In the present case we have  $z = a = 2br$ , and therefore one finds the following explicit formula for Uehling potential  $U(r) = U(2br)$  in position space

$$U(2br) = \frac{2\alpha Q}{3\pi r} \left[ \left(1 + \frac{b^2 r^2}{3}\right) K_0(2br) - \frac{br}{6} Ki_1(2br) + \left(-\frac{b^2 r^2}{3} + \frac{5}{6}\right) Ki_2(2br) \right] , \quad (23)$$

where the notation  $Q$  stands for the electric charge of the nucleus and  $b = \alpha^{-1}$ . Now, Eq.(13) takes the form

$$\begin{aligned} ec\phi(r) &= \frac{Q}{r} \left\{ 1 + \frac{2\alpha}{3\pi} \cdot \left[ \left(1 + \frac{r^2}{3\alpha^2}\right) K_0\left(\frac{2r}{\alpha}\right) - \frac{r}{6\alpha} Ki_1\left(\frac{2r}{\alpha}\right) + \left(\frac{5}{6} - \frac{r^2}{3\alpha^2}\right) Ki_2\left(\frac{2r}{\alpha}\right) \right] \right\} \\ &= \frac{Q}{r} + U(r) \quad (24) \end{aligned}$$

This is the general form of the Coulomb interaction energy between electric charges  $Qe$  and  $e$  which includes the lowest-order vacuum polarization correction. As expected this expression depends only upon the fine structure constant, i.e. upon the  $\hbar$  and  $c$  universal constants and electric charge  $e$  (and  $Qe$ ), but it does not include any particle's mass. The generalization of these formulas to the case of two interacting electric charges  $q_1$  and  $q_2$  is obvious and simple. Note also that the two limiting forms of the Uehling potential mentioned above (see, Section II) which correspond to the cases when  $r \ll \alpha a_0 = \Lambda_e$  and  $r \gg \alpha a_0 = \Lambda_e$ , respectively, can be obtained from these expressions Eqs.(23) - (24).

Note that the formula Eq.(23) includes only three different terms each of which contain either the modified Bessel function of zero order  $K_0(2br)$ , or one of the two recursive integrals from this function, i.e. the  $Ki_1(2br)$  and/or  $Ki_2(2br)$  functions. The formula, Eq.(23),



has many advantages for theoretical analysis as well as for numerical computations. Indeed, the parameter  $b$  in this formula equals  $\alpha^{-1}(\gg 1)$ , and therefore, Eq.(23) can be used to obtain various approximate formulas for the Uehling potential. Each term in such formulas has a different order upon the fine structure constant  $\alpha$  (or  $\alpha^{-1}$ ). Moreover, this closed (and relatively simple) analytical formula is useful in many other problems, e.g., to perform secondary quantization of Maxwell equations which already include vacuum polarization correction. In numerical computations the formula, Eq.(23), allows one to avoid very painful and time-consuming procedures of numerical integration. Briefly, this means that each matrix elements of the Uehling potential is computed analytically in an arbitrary, in principle, basis of radial few-body functions. The closed analytical formulas cannot lead to the loss of numerical accuracy in computations. Furthermore, in this case we do not need to investigate the convergence of the matrix elements and overall results upon various parameters arising in the methods used for numerical integration.

#### IV. RESULTS AND DISCUSSION

To check our analytical formula, Eq.(23), for the Uehling potential we determine the corrections to the bound state energies of some atoms and ions associated with such a potential. In other words, we determine the lowest order vacuum polarization correction(s) for some simple (two-electron) atoms and ions. In general, to evaluate the correction to the bound state energy associated with the Uehling potential one needs to solve the non-relativistic Schrödinger equation for an atomic system with the pure Coulomb potential to very high accuracy. At the second stage of the procedure the non-relativistic wave functions are used to compute the expectation values of the Uehling potential. Formally, in this approach we have to consider the corrections which correspond to all levels of the perturbation theory, e.g., the lowest-order corrections, second-order corrections, etc. The convergence of such series from perturbation theory is often a very complex question. An alternative method is based on the direct solution of the non-relativistic Schrödinger equation with the new interaction potential which includes the Uehling potential. The corresponding correction is determined as a difference of the two energies (eigenvalues) obtained from the solution of the two Schrödinger equations: one of these equations contains the pure Coulomb interaction potential, while in the second equation the interaction potential is represented as a

sum of Coulomb and Uehling potentials. The wave function obtained in the result of the numerical solution of the Schrödinger equation already contains all corrections related with the vacuum polarization correction. By using this method below we determine the vacuum polarization corrections (or Uehling correction) for the two-electron helium atoms and for some helium-like ions.

In our calculations we have used the highly accurate variational wave functions constructed from the exponential basis functions of three relative coordinates  $r_{32}, r_{31}$  and  $r_{21}$ . Each of these trial wave function includes 400 terms (exponents) with the carefully optimized non-linear parameters (more detail about exponential basis functions can be found, e.g., in [15] and references therein). Finally, these trial wave functions for each two-electron atomic system have very good numerical accuracy. It provides  $\approx 12 - 14$  stable decimal digits in the total energy. It is clear that such an accuracy is sufficient to evaluate the lowest order vacuum polarization correction directly and to high accuracy. The results of numerical evaluations of the vacuum polarization correction for the  $^\infty\text{He}$ ,  $^4\text{He}$  and  $^3\text{He}$  atoms can be found in Table I. Our results in Table I include the non-relativistic Coulomb energies  $E_{nr}$  computed with  $N = 400$  basis wave functions and  $N = 4000$  basis functions (exponents) [16]. The last values are designated in Table I as  $E_{nr}(\infty)$ , since it is very close to the exact answer. Table I also includes the total vacuum polarization correction  $\Delta E_{ueh}$  for all three interparticle (Coulomb) interactions in the He atoms. We also determine the vacuum polarization corrections for the electron-nucleus and electron-electron interactions separately. They are designated in Table I as  $\Delta E_{ueh}^{eN}$  and  $\Delta E_{ueh}^{ee}$ , respectively.

As follows from the results of Table I, the overall correction to the energy due to inclusion of the vacuum polarization correction for the two-electron He atom is relatively small  $\approx -7.2555 \cdot 10^{-7} \text{ a.u.}$ . However, such a difference can easily be detected in modern high-precision optical experiments. The contribution of the vacuum polarization correction for the electron-electron interaction is substantially smaller  $\approx -1.1051 \cdot 10^{-8} \text{ a.u.}$ . In other words, in the first approximation we can neglect the correction for the electron-electron interactions in all few-electron atoms. Another interesting fact, which follows from Table I, is the mass dependence of the corrections. The influence of variations in the masses of the helium atom(s)  $^\infty\text{He}$ ,  $^4\text{He}$  and  $^3\text{He}$  appears in the 4th decimal digit in the vacuum polarization correction.

The results of numerical computations of the lowest order vacuum polarization corrections in some two-electron ions can be found in Table II. In Table II we consider the ground

$1^1S(L=0)$ —states of the  $^\infty\text{Li}^+$ ,  $^\infty\text{Be}^{2+}$ ,  $^\infty\text{B}^{3+}$  and  $^\infty\text{C}^{4+}$  ions. Vacuum polarization corrections  $\Delta E_{ueh}$  have been determined for each of these ions and shown in Table II in atomic units. As follows from Table II the vacuum polarization correction rapidly increases with the nuclear charge  $Q$ . Note that our results for the lowest order vacuum polarization correction(s) computed for the ground state of the He atom coincide well with the results of earlier studies (see, e.g., [17] and references therein). In the future work we are planning to apply the formula, Eq.(23), to few-electron atoms and ions. The matrix elements of the Uehling potential must be obtained in different systems of radial basis functions known for few-body systems. Another interesting problem is to compare the efficiency of our method based on the analytical formula, Eq.(23), for the Uehling potential with the methods based on the numerical integration. In particular, such a comparison can be made for the two-electron atomic systems discussed above.

## V. CORRECT ASYMPTOTICS AT LARGE DISTANCES

Our analytical formula for the interaction potential between the electron and atomic nucleus (with the electric charge  $Qe$ ) is written in the following form (in atomic units  $\hbar = 1, m_e = 1$  and  $e = 1$ )

$$\phi(r) = \frac{Q}{r} \left\{ 1 + \frac{2\alpha}{3\pi} \cdot \left[ \left( 1 + \frac{r^2}{3\alpha^2} \right) K_0\left(\frac{2r}{\alpha}\right) - \frac{r}{6\alpha} K_{i_1}\left(\frac{2r}{\alpha}\right) + \left( \frac{5}{6} - \frac{r^2}{3\alpha^2} \right) K_{i_2}\left(\frac{2r}{\alpha}\right) \right] \right\} \\ = \frac{Q}{r} + U(r) \quad (25)$$

where  $U(r)$  is the Uehling potential,  $K_0(z)$  is the modified Bessel function of zero order, while  $K_{i_1}(z)$  and  $K_{i_2}(z)$  are the recursive integrals of the  $K_0(z)$  function (see above). Note that the formula, Eq.(25), is correct mathematically, but it has a wrong ‘physical’ asymptotic at large distances  $r$ , e.g., at  $r \geq 10\alpha a_0$ , where  $a_0 = \frac{\hbar^2}{m_e e^2}$  is the Bohr radius. First, note that the short range asymptotic of the  $\phi(r)$  potential, Eq.(24), takes the form

$$\phi(r) |_{r \rightarrow 0} \simeq \frac{Q}{r} \left\{ 1 + \frac{\alpha}{3\pi} \left[ -\frac{5}{3} - 2\gamma + 2 \ln \alpha - 2 \ln r \right] \right\} \quad (26)$$

where  $\gamma \approx 0.5772156649 \dots$  is the Euler constant (see, e.g., [11]) and  $\ln \alpha \approx -4.92024365857$ . The long-range asymptotics of the potential  $\phi(r)$ , Eq.(24), is (in atomic units)

$$\phi(r) |_{r \rightarrow \infty} \simeq \frac{Q}{r} \left\{ 1 + \frac{\alpha^{\frac{5}{2}}}{4\sqrt{\pi} r^{\frac{3}{2}}} \exp\left(-\frac{2}{\alpha} r\right) \right\} \quad (27)$$

This means that the long-range asymptotics of  $\phi(r)$  decreases with  $r$  exponentially. This is not correct physically, since the exponential function vanishes at  $r \rightarrow +\infty$  very rapidly. In reality, such an incorrect asymptotics of the interaction potential  $\phi(r)$  at large distances  $r$  is overweighted by the lowest order QED correction to the electromagnetic field ( $\mathbf{E}, \mathbf{H}$ ), or to the pure electric field  $\mathbf{E}$  in our case, when  $\mathbf{H} = 0$ . This correction provides the correct power-type dependence of the interparticle potential at large distances. It is directly related to the non-linearity of the Maxwell equation for the EM-field [5], [18].

By following the method used in [18] let us obtain the lowest order QED correction to the pure electric field  $\mathbf{E}$ . Consider one point electric charge located at the center of coordinates  $x = 0, y = 0, z = 0$ . This charge is assumed to be at rest. The corresponding Lagrangian  $L$  which includes the lowest order QED correction is written in the form (in regular units)

$$L = \frac{1}{2}\mathbf{E}^2 + \frac{e^4\hbar}{360\pi^2m_e^4c^7}\mathbf{E}^4 = \frac{1}{2}(\nabla\phi)^2 + \frac{e^4\hbar}{360\pi^2m_e^4c^7}(\nabla\phi)^4 = L[\phi(r)] \quad (28)$$

where  $\mathbf{E} = -\nabla\phi(r)$ . By varying the potential  $\phi(r)$  in the equation (the fundamental equation of least action) [18]

$$\delta \int L[\phi(r)]r^2dr = 0 \quad (29)$$

one finds the following differential equation

$$\frac{d\phi}{dr} + \frac{e^4\hbar}{90\pi^2m_e^4c^7}\left(\frac{d\phi}{dr}\right)^3 = \frac{C}{r^2} \quad (30)$$

where  $C = -\frac{Qe}{4\pi}$ . Assuming that  $\phi(r) = \frac{Qe}{4\pi r} + \psi(r)$ , where  $\psi(r)$  is a very small correction to the Coulomb potential, we reduce the last equation to the form

$$\frac{d\psi}{dr} = \frac{e^4\hbar}{90\pi^2m_e^4c^7}\left(\frac{Q^3e^3}{64\pi^3r^6}\right) \quad (31)$$

From this equation one finds

$$\psi(r) = -\frac{e^7\hbar}{450\pi^2m_e^4c^7}\left(\frac{Q^3}{64\pi^3r^5}\right) \quad (32)$$

Therefore, the total interaction potential  $\phi(r)$  is

$$\phi(r) = \frac{Qe}{4\pi r} - \frac{e^7\hbar}{450\pi^2m_e^4c^7}\left(\frac{Q^3}{64\pi^3r^5}\right) = \frac{Qe}{4\pi r}\left[1 - \frac{2\hbar}{225\pi m_e^4c^7}\left(\frac{Q^2e^6}{64\pi^3}\right)\frac{1}{r^4}\right] \quad (33)$$

In the relativistic units  $\hbar = 1, c = 1$  and  $\alpha = \frac{e^2}{4\pi}$  the last formula takes the form

$$\phi(r) = \frac{Qe}{4\pi r}\left[1 - \frac{2Q^2\alpha^3}{225\pi m_e^4r^4}\right] \quad (34)$$

This expression is the sum of the Coulomb potential and small correction which exactly coincides with the well known Wichmann-Kroll potential [18]. In atomic units the last expression is

$$\phi(r) = \frac{Q}{r} \left[ 1 - \frac{2Q^2\alpha^7}{225\pi r^4} \right] = \frac{Q}{r} - \frac{2Q^3\alpha^7}{225\pi r^5} \quad (35)$$

and Wichmann-Kroll potential  $W_K(r)$  is

$$\psi(r) = W_K(r) = -\frac{2Q^3\alpha^7}{225\pi r^5} \quad (36)$$

Note that this potential is not regular at the origin. However, as follows from the Appendix such a singularity is formal, since Eq.(30) is not correct at  $r \rightarrow 0$  (see Appendix). It can be removed by using the substitution  $r \rightarrow r + \alpha$  in atomic units or  $r \rightarrow r + \alpha a_0$  in regular units. This substitution removes singularity of the  $W_K(r)$  potential at  $r = 0$  and changes its behaviour at short interparticle distances  $r \leq \alpha$ . However, at such distances the Wichmann-Kroll correction is not important and its contribution is significantly smaller than contribution from the Uehling potential. On the other hand, at large distances, i.e. for  $r \geq 10\alpha a_0$  (and even for  $r \geq \alpha a_0$ ) the contribution from the Wichmann-Kroll potential plays the leading role. Finally, we can write the correct expression for the Wichmann-Kroll potential  $W_K(r)$

$$\psi(r) = W_K(r) = -\frac{2Q^3\alpha^7}{225\pi(r + \alpha)^5} \quad (37)$$

Note that this potential is always negative. In general, at  $r \approx a_0$  this potential is very small by its absolute value. However, its overall contribution rapidly increases with the nuclear charge  $Q$ . Furthermore, it decreases with the distance  $r$  as  $\sim r^{-5}$ , i.e. non-exponentially. It is clear that at some large distance the Wichmann-Kroll correction will always exceed the contribution from the Uehling potential  $U(r)$ , Eq.(24). Thus, the following interaction potential (in atomic units) of the two point electric charges

$$\begin{aligned} \Phi(r) = \frac{Q}{r} + U(r) + W_K(r) = \frac{Q}{r} + \frac{2Q\alpha}{3\pi r} \cdot \left[ \left( 1 + \frac{r^2}{3\alpha^2} \right) K_0\left(\frac{2r}{\alpha}\right) - \frac{r}{6\alpha} K_1\left(\frac{2r}{\alpha}\right) \right. \\ \left. + \left( \frac{5}{6} - \frac{r^2}{3\alpha^2} \right) K_2\left(\frac{2r}{\alpha}\right) \right] - \frac{2Q^3\alpha^7}{225\pi(r + \alpha)^5} \end{aligned} \quad (38)$$

has the correct asymptotic behaviour both at small and large interparticle distances. In the case of interaction between two point electric charges  $q_1e$  and  $q_2e$  we need to replace in Eq.(38) the factor  $Q$  by the product  $q_1q_2$ . The potential  $\Phi(r_{12})$  takes the form

$$\Phi(r_{12}) = \frac{q_1q_2}{r_{12}} + \frac{2q_1q_2\alpha}{3\pi r_{12}} \cdot \left[ \left( 1 + \frac{r_{12}^2}{3\alpha^2} \right) K_0\left(\frac{2r_{12}}{\alpha}\right) - \frac{r_{12}}{6\alpha} K_1\left(\frac{2r_{12}}{\alpha}\right) \right. \\ \left. + \left( \frac{5}{6} - \frac{r_{12}^2}{3\alpha^2} \right) K_2\left(\frac{2r_{12}}{\alpha}\right) \right] - \frac{2q_1^3\alpha^7}{225\pi(r_{12} + \alpha)^5}$$

$$+\left(\frac{5}{6}-\frac{r_{12}^2}{3\alpha^2}\right)Ki_2\left(\frac{2r_{12}}{\alpha}\right)\Big]-\frac{2(q_1q_2)^3\alpha^7}{225\pi(r_{12}+\alpha)^5} \quad (39)$$

where  $r_{12}$  is the distance between particles 1 and 2.

Thus, we have derived the formula for the interaction between two point electric charges which includes the lowest order QED corrections to the Coulomb potential. Our formulas, Eqs.(38) - (39), provide the correct asymptotic behaviour at arbitrary interparticle distances. The formulas, Eqs.(38) - (39), can directly be used in highly accurate computations of the bound states in few-electron atoms and ions. The explicit computation of the electric field strength  $\mathbf{E}$ , i.e. the spatial gradient from the  $\Phi(r_{12})$  potential, Eq.(39), is straightforward, but the Fourier resolution of the corresponding ‘electrostatic’ field is extremely complicated. Note also that for the potential  $\Phi(r)$ , Eq.(38), the condition  $\Delta\Phi(r) = 4\pi Q\delta(\mathbf{r})$ , where  $\Delta = \nabla \cdot \nabla = \text{div}(\text{grad}...)$ , is not obeyed.

## VI. CONCLUSION

Thus, we have derived the closed analytical expression for the Uehling potential which represents the lowest order vacuum polarization correction(s) in atomic systems. It is shown that the Uehling potential can be represented as a sum of the modified Bessel function of the zero order  $K_0(2br)$  and the recursive integrals of this function, i.e. the  $Ki_1(2br)$  and  $Ki_2(2br)$  functions (see Eq.(23)). Based on our explicit and relatively simple three-term formula, Eq.(23), we can reject a well known existing conclusion that the Uehling potential cannot be represented by the closed analytical formula. Moreover, we have found that such a simple analytical formula drastically simplifies theoretical analysis of vacuum polarization in light atoms and ions. Numerical algorithms based on this formula are usually very fast and effective for accurate calculations of atomic systems. Briefly, we can say that the use of this closed analytical formula for the Uehling potential opens a new avenue in investigation of the vacuum polarization in light and heavy atoms and ions and muonic atoms and ions. It can be used for various theoretical purposes, e.g., to perform secondary quantization of Maxwell equations modified to the form which includes the lowest order vacuum polarization correction.

To check our analytical formula for the Uehling potential, Eq.(23), we have determined the lowest order vacuum polarization correction for some atoms and ions. In particular,

these corrections are evaluated numerically for the ground  $1^1S$ -states of the two-electron He atoms and He-like ions. The overall contribution from vacuum polarization for He-atoms is evaluated as  $\approx -7.2555 \cdot 10^{-7} \text{ a.u.}$  The main contribution to this correction comes from electron-nucleus interactions. The effect of vacuum polarization for the electron-electron interactions is very small (at least by an order of magnitude smaller) and can be neglected in the lowest-order approximation. We also determine the vacuum polarization correction for some two-electron (or helium-like) ions. In particular, we have determined such corrections for the ground  $1^1S$ -states in the  $\text{Li}^+$ ,  $\text{Be}^{2+}$ ,  $\text{B}^{3+}$  and  $\text{C}^{4+}$  ions.

We also derived the general formula, Eq.(39), for the interaction between two point electric charges. This expression includes the lowest order QED corrections to the regular Coulomb potential. Our formulas, Eqs.(38) - (39), have the correct asymptotic behaviour at small and large interparticle distances. Briefly, we can consider this formula as the modified Coulomb potential which agrees with the rules of modern QED in the lowest order.

### Acknowledgements

It is a pleasure to acknowledge the University of Western Ontario for financial support. One of us (AMF) wants to thank Professor Joachim Reinhardt (Frankfurt, Germany) for his help with Eqs.(23) and (24).

### Appendix

The equation, Eq.(30), is a cubic equation in respect to the radial derivative of the unknown potential  $\psi(r)$ . It can be re-written in the form

$$\frac{e^4 \hbar}{90\pi^2 m_e^4 c^7} y^3 + y + \frac{Qe}{4\pi r^2} = 0 \quad (40)$$

where  $y = \frac{d\psi}{dr}$ . As follows from the general theory of cubic functions this equation has only one real root (the discriminant of this equation is negative). In fact, this equation is easily reduced to the form of a monic trinomial (see, e.g., [19])

$$y^3 + py + \frac{q}{r^2} = 0 \quad (41)$$

where  $p = \frac{90\pi^2 m_e^4 c^7}{e^4 \hbar}$  and  $q = \frac{45\pi Q m_e^4 c^7}{2e^3 \hbar}$ .

The Cardano method gives the only real root of Eq.(41)

$$y = \sqrt[3]{-\frac{q}{2r^2} + \sqrt{\frac{q^2}{4r^4} + \frac{p^3}{27}}} + \sqrt[3]{-\frac{q}{2r^2} - \sqrt{\frac{q^2}{4r^4} + \frac{p^3}{27}}} \quad (42)$$

In other words, we obtain the following differential equation

$$\frac{d\phi}{dr} = \sqrt[3]{-\frac{q}{2r^2} + \sqrt{\frac{q^2}{4r^4} + \frac{p^3}{27}}} + \sqrt[3]{-\frac{q}{2r^2} - \sqrt{\frac{q^2}{4r^4} + \frac{p^3}{27}}} \quad (43)$$

At  $r \rightarrow \infty$  this equation has the solution  $\psi(r) = 2(\frac{p}{3})^{\frac{1}{2}} \cdot r + B$ , where  $B$  is some numerical constant. Such an asymptotics is not correct. At  $r \rightarrow 0$  the analogous solution takes the form  $\psi(r) = -3q^{\frac{1}{3}} \cdot r^{\frac{1}{3}} + C$ , where  $C$  is some numerical constant. The numerical constant  $C$  must contain the fine structure constant  $\alpha$ . The overall contribution of the Wichmann-Kroll term at small  $r$  must be smaller than the analogous contribution from the Uehling potential. This gives  $C \simeq \alpha^n$ , where  $n \geq 2$ . Now, it is easy to check that the substitution  $r \rightarrow r + \alpha$  (or  $r \rightarrow r + \alpha a_0$ ) used in the main text is indeed the correct way to regularize the Wichmann-Kroll potential at small  $r$ .

- 
- [1] P.A.M. Dirac, *Lectures on Quantum Mechanics.*, (Yeshiva University, New York, (1964)).
  - [2] W. Heisenberg and H. Euler, Z. Physik **38**, 314 (1936).
  - [3] W. Pauli and F. Villars, Rev. Mod. Phys. **21**, 434 (1949).
  - [4] W. Greiner, *Relativistic Quantum Mechanics. Wave equations.* (3rd. Ed., Springer Verlag, Berlin, (2000)), p. 252.
  - [5] A.I. Akhiezer and V.B. Berestetskii, *Quantum Electrodynamics*, (Interscience, New York (1965)).
  - [6] E.A. Uehling, Phys. Rev. **48**, 55 (1935).
  - [7] W. Pieper and W. Greiner, Nucl. Phys. A **109**, 539 (1968).
  - [8] G. Plunien and G. Soff, Phys. Rev. A **51**, 1119 (1995).
  - [9] W. Heitler, *The Quantum Theory of Radiation* (3rd. ed., Oxford at the Clarendon Press, Oxford (1954)).
  - [10] The NIST Reference on Constants, Units and Uncertainty, (see: <http://physics.nist.gov/cuu/Constants/index.html>)
  - [11] I.S. Gradshteyn and I.M. Ryzhik, *Tables of Integrals, Series and Products*, (5th ed., Academic Press, New York, (1994)).
  - [12] E.H. Wichmann and N.M. Kroll, Phys. Rev. **101**, 843 (1956).



- [13] W. Greiner and J. Reinhardt, *Quantum Electrodynamics* (3rd. Ed., Springer Verlag, Berlin (2003)).
- [14] *Handbook of Mathematical Functions*, M. Abramowitz and I.A. Stegun, eds. (Dover, New York, (1972)).
- [15] A.M. Frolov, Phys. Lett. A **350**, 241 (2006).
- [16] A.M. Frolov, J. Chem. Phys. **126**, 104302 (2007); *ibid*, **124**, 224323 (2006).
- [17] L. Wayne Fulleton and G.A. Rinker, Phys. Rev. A **13**, 1283 (1976).
- [18] E.H. Wichmann and N.M. Kroll, Phys. Rev. **101**, 843 (1956).
- [19] *Handbook of Mathematical Functions*, M. Abramowitz and I.A. Stegun, eds. (Dover, New York, (1972)).

TABLE I: The total non-relativistic energies  $E_{nr}(400)$  of the ground  $1^1S(L=0)$ -state of the  $^\infty\text{He}$ ,  $^4\text{He}$  and  $^3\text{He}$  atom and vacuum polarization corrections (in atomic units).

atom	$^\infty\text{He}$	$^4\text{He}$	$^3\text{He}$
$E_{nr}(\infty)$	-2.9037243770341195831	-2.9033045577295687858	-2.9031672107105772470
$E_{nr}(400)$	-2.90372437703405	-2.90330455772950	-2.90316721071051
$\Delta E_{ueh}$	$-7.255456205 \cdot 10^{-7}$	$-7.252434438 \cdot 10^{-7}$	$-7.251448021 \cdot 10^{-7}$
$\Delta E_{ueh}^{eN}$	$-7.366031256 \cdot 10^{-7}$	$-7.362968355 \cdot 10^{-7}$	$-7.361966472 \cdot 10^{-7}$
$\Delta E_{ueh}^{ee}$	$1.10575051 \cdot 10^{-8}$	$1.10533917 \cdot 10^{-8}$	$1.10518451 \cdot 10^{-8}$

The energies  $\Delta E_{ueh}^{eN}$  include the vacuum polarization correction for the electron-nucleus

interactions only, i.e.  $\Delta E_{ueh}^{eN} = \Delta E_{ueh} - \Delta E_{ueh}^{ee}$ .

TABLE II: The total non-relativistic energies  $E_{nr}(400)$  of the ground  $1^1S(L=0)$ -state of the  $^\infty\text{Li}^+$ ,  $^\infty\text{Be}^{2+}$ ,  $^\infty\text{B}^{3+}$ ,  $^\infty\text{C}^{4+}$ , and vacuum polarization corrections (in atomic units).

ion	$^\infty\text{Li}^+$	$^\infty\text{Be}^{2+}$	$^\infty\text{B}^{3+}$	$^\infty\text{C}^{4+}$
$E_{nr}(\infty)$	-7.27991341266930596	-13.65556623842358670	-22.03097158024278154	-36.40624660189853031
$E_{nr}(400)$	-7.27991341266315	-13.6555662384085	-22.0309715801925	-36.4062466018083
$\Delta E_{ueh}$	$-2.706070460 \cdot 10^{-6}$	$-6.714805549 \cdot 10^{-6}$	$-1.342648935 \cdot 10^{-5}$	$-2.349488675 \cdot 10^{-5}$
$\Delta E_{ueh}^{eN}$	$-2.762425832 \cdot 10^{-6}$	$-6.873080812 \cdot 10^{-6}$	$-1.377060071 \cdot 10^{-5}$	$-2.413281437 \cdot 10^{-5}$
$\Delta E_{ueh}^{ee}$	$5.6355372 \cdot 10^{-8}$	$1.5927526 \cdot 10^{-7}$	$3.4412136 \cdot 10^{-7}$	$6.3792762 \cdot 10^{-7}$

The energies  $\Delta E_{ueh}^{eN}$  include the vacuum polarization correction for the electron-nucleus

interactions only, i.e.  $\Delta E_{ueh}^{eN} = \Delta E_{ueh} - \Delta E_{ueh}^{ee}$ .